

Novel glassy behavior in a ferromagnetic p-spin model

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Recent work has suggested the existence of glassy behavior in a ferromagnetic model with a four-spin interaction. Motivated by these findings, we have studied the dynamics of this model using Monte Carlo simulations with particular attention being paid to two-time quantities. We find that the system shares many features in common with glass forming liquids. In particular, the model exhibits: (i) a very long-lived metastable state, (ii) autocorrelation functions that show stretched exponential relaxation, (iii) a non-equilibrium timescale that appears to diverge at a well defined temperature, and (iv) low temperature aging behaviour characteristic of glasses.

I. INTRODUCTION

Many liquids when cooled below the melting temperature do not crystallize. Instead, as the temperature is lowered, the relaxation time (or the viscosity) increases dramatically, eventually becoming so large that the liquid appears frozen on experimental timescales. For all practical purposes the system has solidified yet there is no long range order. The system is said to have become a glass. Despite over fifty years of work, a consensus is lacking on a theory of this phenomenon [1]. Even as basic a question as the existence of a genuine thermodynamic glass transition is difficult to decide experimentally. Therefore, much work in this field has been numerical. Simulations in the continuum of glassy systems remain difficult, and, despite the substantial progress in this direction [2], there are still many unresolved issues.

Because of these problems it would be useful to have simplified lattice models that behave in some respects like glasses and which do not have quenched disorder. Recently, Lipowski [3] and Lipowski and Johnston [4,5] studied such a model by Monte Carlo simulations and provided evidence of glassy behavior. The model is defined by the Hamiltonian

$$H = -J \sum_{\square} S_i S_j S_k S_l, \quad (1)$$

where the spins sit on a cubic lattice and the interactions are between the four spins at the corners of each plaquette. The spin variables take values $S_i = \pm 1$ and J is the strength of the ferromagnetic coupling. (We will take $J = 1$ in all that follows.) Their study was motivated by the fact that the spin-glass version of this model was found numerically [6] to have several features in common with structural glasses. In addition, there is a close connection [3] between the plaquette model, Eq. 1, and the

Ising model with competing interactions studied in the context of glasses by Shore and Sethna [7]. Lipowski and Johnston [4] showed that, in equilibrium, the plaquette model has a first order transition as the temperature is lowered but that this transition is never observed in simulations within accessible timescales. Instead, one sees what appears to be a dynamical transition to a glassy state [4,5].

The work of these authors concentrated on single time quantities. To see clear signatures of glassy behaviour and to understand which particular aspects of glasses are present in this model, it is important to study two time quantities such as autocorrelation and response functions. We do just that in this paper and our findings are organized as follows: in section II, we summarize the results of Lipowski and Johnston on the statics of the plaquette model and the strong metastability that they observed. In section III, we examine the metastable state in greater detail. In particular, we calculate the timescale for nucleation and show that it is indeed extremely large. In section IV, we present results for the energy auto-correlation function in the supercooled phase which is unambiguously described by a stretched exponential. We investigate the behavior of the associated timescale as a function of temperature, showing that it diverges with a power law at a temperature indistinguishable from the lower limit of metastability. This temperature is that which the authors of [3,4] called the glass transition temperature T_g . In section V, we study the dynamical behavior below T_g . The spin-spin autocorrelation function and overlap distribution function exhibit aging of a form that is characteristic of glasses, showing that the plaquette model has a complex free-energy landscape. These findings provide further evidence to support the conjecture that the plaquette model exhibits an ideal glass transition.

II. THE PLAQUETTE MODEL

In equilibrium, the model defined by Eq. 1 has a first order transition at $T_c \simeq 3.6$ [4, 8, 9]. This system possesses a novel symmetry: flipping all the spins in any plane of the cubic lattice leaves the Hamiltonian invariant, leading to a degeneracy of ground states $\sim 2^{dL}$ for a cubic system of size L in d dimensions. Note, however, that the ground state entropy is finite. Because of this symmetry, the magnetisation is not a good order parameter. Instead, one can use the internal energy per spin, E , to investigate this model further.

Lipowski and Johnston looked at the dynamics of E following a quench from a high temperature state to a temperature $T < T_c$ [4]. They found different behaviour depending on the value of T . In particular, for $3.4 < T < T_c$, E appears not to relax to its value in the low temperature phase. Rather it settles into a plateau at an energy higher than that of the true low temperature phase at the same temperature. Furthermore, the time the system spends on the plateau (in a “supercooled” state) appears to increase at least exponentially with system size, suggesting the existence of a genuine metastable phase. Such behaviour, if present, would indeed be strange because one does not expect true metastability (i.e. two local minima of the free energy separated by diverging free energy barriers) in systems with finite range interactions. Moreover, nucleation theory tells us that the larger the system, the shorter the lifetime of a metastable state, provided that the system is large enough to support a nucleating droplet. To understand whether the strong metastability is indeed a finite size artifact, Lipowski and Johnston studied a quench starting from a configuration with a droplet of the low temperature phase in a high temperature background. They reported that for sufficiently large seeds, the system always relaxed to the low temperature phase, concluding that ordinary nucleation was operative. However, this does not explain why the supercooled phase appears so stable on observable timescales. The analysis we report in the next section provides an explanation for this phenomenon.

For quenches to below $T = 3.4$ the behaviour was found to be quite different. The plateau disappeared and, after initial transients, the energy decreased extremely slowly. Moreover, it appeared to relax not to the value in the low temperature phase, but to a value extensively higher. They identified this state as the glassy phase. Finally, they have recently shown that a characteristic zero-temperature length increases very slowly with the inverse cooling rate, as is seen in ordinary glasses [5].

To summarize, this model has many properties that are similar to those seen in real glasses: a first order transition analogous to crystal melting, strong metastability effects in the supercooled phase, and a kinetic transition to a glassy state characterised by slow dynamics.

In the next section we will discuss the anomalous

metastability described above before looking in some detail at the dynamical behavior of this model by studying the autocorrelation functions both in the supercooled phase and in the “glassy” state.

III. METASTABILITY

We begin by summarizing the basics of nucleation theory [10]. The idea is that if the system is in a metastable state, the process of finding the true free-energy minimum involves the formation of a droplet of the stable phase which can grow and take over the whole system. Phenomenologically, one can express the free energy barrier to forming a droplet of linear dimension R as $\Delta = A\sigma R^{d-1} - B\delta f R^d$ in d dimensions. Here σ is the surface tension between the metastable and stable phases and δf is the difference in the bulk free energy densities of the two phases. A and B are constants characterizing the geometrical shape of the droplet. Because the surface term is a cost and the bulk term is a gain, one can maximize Δ to find a critical radius $R^* = (A(d-1)/Bd)(\sigma/\delta f)$. Droplets of a radius greater than R^* can grow and take over the whole systems while those of radius less than R^* will shrink. At low temperatures and in three dimensions, the timescale for nucleation of a droplet is then given by $\tau_{\text{nuc}} \sim \exp(4A^3\sigma^3/27B^2\delta f^2T)$.

For the plaquette problem, the free energy difference between the two phases can be estimated from the data in [4]. We find $\delta f \approx 0.5|T - T_c|$. The surface tension σ at T_c can be calculated from the size dependence of the mean time it takes the system to flip between the high and low temperature phases. This time τ_{flip} is given by $\tau_{\text{flip}} \sim e^{2\sigma L^2/T_c}$, where L is the system size and the factor of 2 comes from using periodic boundary conditions. We have performed standard single spin-flip Monte Carlo simulations to determine this transition time numerically for systems of size $L = 4, 5, 6, 7, 8$. The transitions are identified from jumps in the energy between the values appropriate to the high and low temperature phases. For each system size, an ‘effective transition temperature’, $T_c(L)$, is determined by the requirement that the system spend equal time in both phases, i.e. at each of the two possible values of the energy. This gives $T_c(L) \simeq 4.45, 4.19, 4.03, 3.92$ and 3.86 for $L = 4, 5, 6, 7$ and 8 respectively. The mean transition time, $\tau_{\text{flip}}(L)$, is measured at $T_c(L)$, and the surface tension, σ , obtained by plotting $\ln \tau_{\text{flip}}(L)$ against $L^2/T_c(L)$. The data is presented in Fig. 1. For large L , the points should approach a straight line with slope 2σ . Since there is clear curvature in the data for the small values of L available, we attempt an extrapolation to large L by plotting $[T_c(L)/L^2] \ln \tau_{\text{flip}}$ against $T_c L/L^2$, as shown in the inset to Fig. 1. The intercept on the vertical axis gives 2σ . While the extrapolation to $L = \infty$ is necessarily subjective, from the curvature of the data it is clear that any reasonable procedure will give a value of 2σ greater than the value $\simeq 0.62$ ob-

tained from a linear extrapolation of the last two points, and less than the value $\simeq 0.69$ given by the $L = 8$ point. To obtain lower bounds on critical drop sizes and nucleation times we use the estimate $\sigma \simeq 0.31$ obtained from the linear extrapolation. Assuming that σ depends only weakly on T close to T_c , and taking $T_c = 3.6$, we estimate the critical droplet radius at $T = 3.5$ to be $R^* \approx 25$ for a cubic droplet ($A = 6$, $B = 1$) and ≈ 12 for a spherical droplet ($A = 4\pi$, $B = 4\pi/3$). The corresponding time to nucleate a cubic droplet is of the order of 10^{47} MCS (and $\sim 10^{25}$ MCS for a spherical droplet).

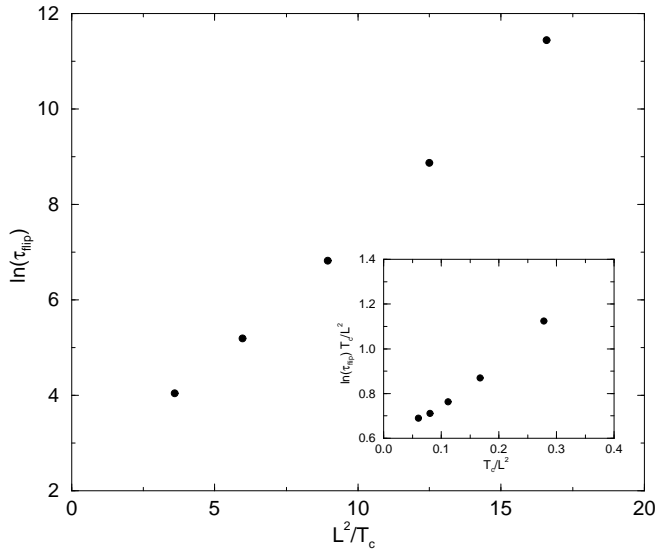


FIG. 1. Logarithm of the flip time between high and low temperature phases at T_c as a function of system size. The errors are smaller than the symbols plotted. The inset shows the extrapolation for large L .

These findings provide an explanation for the results of [4], in which it was noted that the relaxation time of the metastable phase grows rapidly with system size. In [4], the system sizes simulated were all less than, or of the same order as, R^* . In this limit, the free energy barrier to nucleation is set by the system size alone, as a droplet of the equilibrium phase cannot fully form. Consequently, the lifetime of the metastable state will grow exponentially with the size of the system [4] as reported. We thus conclude that the supercooled state is indeed metastable but its lifetime is many orders of magnitude larger than the times accessible in Monte Carlo simulations.

IV. DYNAMICS IN THE SUPERCOOLED PHASE

The philosophy underlying the search for models without disorder that show glassy behavior is that in glasses, inhomogeneities are self-generated, even though the microscopic Hamiltonian has no intrinsic disorder. Thus there is a spontaneous separation of the degrees of free-

dom into variables that exhibit either slow or fast relaxation. One expects that it is the slow degrees of freedom that freeze as the glass transition is approached. However, this separation is not necessarily a priori obvious, and one has to be careful about which quantities one studies. It might happen, for example, that the spin-spin autocorrelations do not show any anomalous behavior, but that some complicated functions of the spins show a dramatic slowing down. For this reason it is often useful to look at autocorrelation functions of global quantities because these presumably pick out the longest timescale or the slowest degree of freedom.

For the system defined by Eq. 1, one such quantity is the energy per spin, E , and we now discuss our findings for the energy autocorrelation function in the range of temperatures $T_g < T < T_c$. Our results have been obtained from Monte Carlo simulations using single spin-flip Glauber dynamics. We have considered cubic systems of linear size L , with L ranging from 12 to 64. Most of the data presented here is for a system size of $L = 48$. To measure the energy autocorrelation function at some temperature T we start from a random configuration (infinite temperature) and quench to the temperature T . We then wait for a time t_w and measure the autocorrelation function $A(t, t_w)$ for subsequent times, t , where $A(t, t_w) = \langle E(t_w)E(t_w + t) \rangle$. The angular brackets denote averages over random initial conditions. In equilibrium one expects $A(t, t_w)$ to be independent of t_w and it is only in equilibrium that one can define a meaningful timescale associated with relaxation. In the supercooled phase, we found that equilibrium is easily achieved in terms of this definition even though the system is in a metastable state. In particular, for any temperature $T_g < T < T_c$, the autocorrelation function becomes independent of t_w once t_w becomes of the order of 10^3 MCS. Note that this time is at least 10 orders of magnitude smaller than the lifetime of this metastable state.

In Fig. 2 we show $A(t, t_w)$ for three different temperatures below T_c and above T_g , together with attempted fits to stretched exponentials of the form

$$A(t, t_w) = A_0 e^{-(\frac{t}{\tau})^\beta}. \quad (2)$$

As can be seen from the figure, the fits are extremely good and we can identify a timescale for relaxation, τ , at each temperature. The exponent β is also temperature dependent and is found to lie in the range $0.5 < \beta < 1$. In Fig. 3 we plot the behaviour of τ as a function of T . It appears to increase sharply as T is reduced and can be fit quite accurately by a power-law divergence,

$$\tau = \frac{2.23}{T - 3.39}, \quad (3)$$

as shown in the figure. This gives a “critical” temperature very close to that which was identified in [4] as the lower limit of stability, T_g , and interpreted as the glass transition temperature. Both stretched exponential relaxation functions and a diverging relaxation time are

features of real glasses. We also tried a Vogel-Fulcher (stretched-exponential) fit to τ but found that the corresponding “critical temperature” is significantly lower than T_g . As we will show in the next section, T_g signifies the onset of aging phenomena and it is thus impossible to define a timescale below this temperature. (We have also measured the spin-spin autocorrelation function but found that the behaviour was much harder to interpret. In fact, the difficulty of interpreting relaxational behavior of local quantities has been noted before in molecular dynamics studies of Lennard-Jones systems in two dimensions [11].)

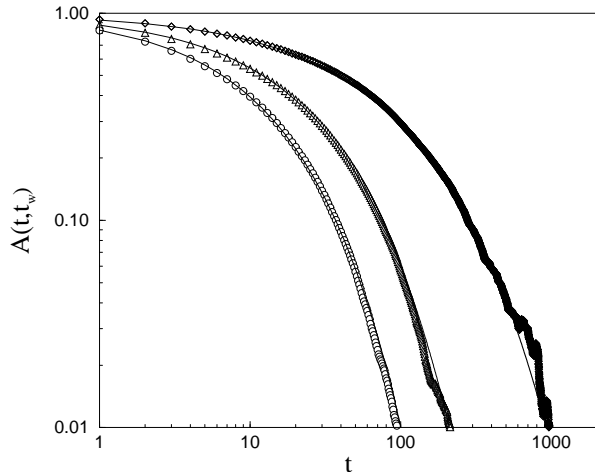


FIG. 2. The energy autocorrelation function $A(t, t_w)$ in the supercooled phase. Three temperatures are shown: $T = 3.6(\circ)$, $3.5(\triangle)$, $3.42(\diamond)$. The lines are fits to stretched exponentials, Eq. 2, with parameters: $\tau = 11, \beta = 0.7$ at $T = 3.6$, $\tau = 21, \beta = 0.66$ at $T = 3.5$ and $\tau = 72, \beta = 0.6$ at $T = 3.42$.

A possible explanation for this divergence is to note that in mean-field theory, the plaquette model has a first order transition at a temperature quite close to T_c [9]. In any mean-field first order transition, one expects a region of metastability delimited by the spinodal temperature. Above this temperature, there is genuine metastability and one expects timescales of autocorrelation functions to diverge as the spinodal temperature is approached. When one moves away from mean-field, genuine metastability is no longer present and instead the spinodal gets rounded out. Our results for the autocorrelation functions, and those of the authors of [4] for the energy relaxation, suggest that the spinodal is actually remarkably well-defined in this short-range system. It is therefore plausible that what we are calling the glass transition temperature is really a remnant of the mean-field spinodal. This too is something that is seen in Lennard-Jones systems in two dimensions [11]. However, the stretched exponential form of $A(t, t_w)$ would not be expected in any simple mean-field treatment.

Thus, the short-range plaquette model has a first order transition analogous to crystal melting, but because

of the extraordinarily long-lived supercooled phase, it also exhibits timescales for relaxation that diverge at T_g . We would like to emphasize that in this model T_g is not strictly well-defined. In fact, we expect that as one gets closer and closer to T_g , or waits for longer in the metastable state, the divergence we are seeing will get rounded out. Numerically, however, it is not possible to see this rounding in any reasonable amount of time. This again is a feature in common with glass forming liquids.

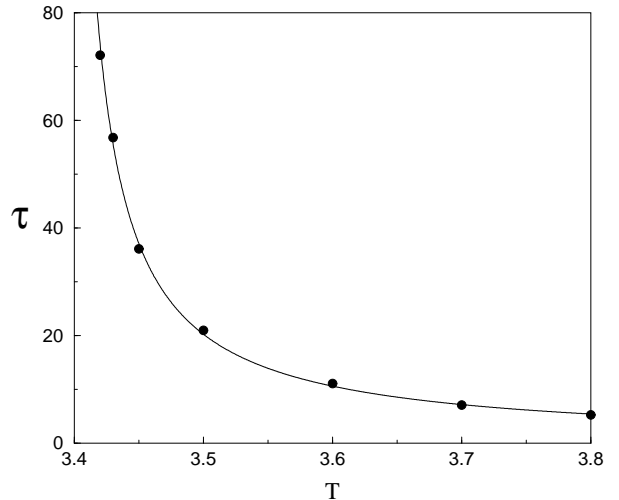


FIG. 3. The timescale of relaxation τ as a function of temperature. The curve is the best fit to a power-law divergence given by Eq. 3.

V. DYNAMICS IN THE GLASSY PHASE

For a quench to a temperature $T > T_g$, as we have seen above, the system becomes trapped in a metastable state for times up to 10^{24} MCS. Within this time window, two-time correlation functions become waiting-time independent and the system behaves as if in equilibrium. This is no longer the case if $T < T_g$. The system now continues to evolve slowly for all accessible times and two-time quantities exhibit aging. To investigate this behaviour we have measured the spin-spin autocorrelation function,

$$C(t, t_w) = \frac{1}{N} \sum_i S_i(t_w) S_i(t + t_w), \quad (4)$$

for a range of waiting-times t_w . Our results are shown in Fig. 4. There is a strong dependence on t_w for all times and temperatures we have considered. In the long time regime, $C(t, t_w)$ decays as a power of t with an exponent of around 0.35. Similar behaviour has been noted in MD simulations of binary Lennard-Jones mixtures [12]. We have also attempted to collapse the data at a fixed temperature with a scaling form $C(t, t_w) = \bar{C}(t/\tau(t_w))$ where $\tau(t_w) \sim t_w^\alpha$. While the fit is not perfect, our best estimate for α is $\alpha = 2$. This type of behaviour has been termed

super-aging [15] as the characteristic timescale for relaxation, $\tau(t_w)$, grows faster than the weighting time itself. Note that the spin-glass version of this model exhibits sub-aging with $\alpha \approx 0.77$ [6].

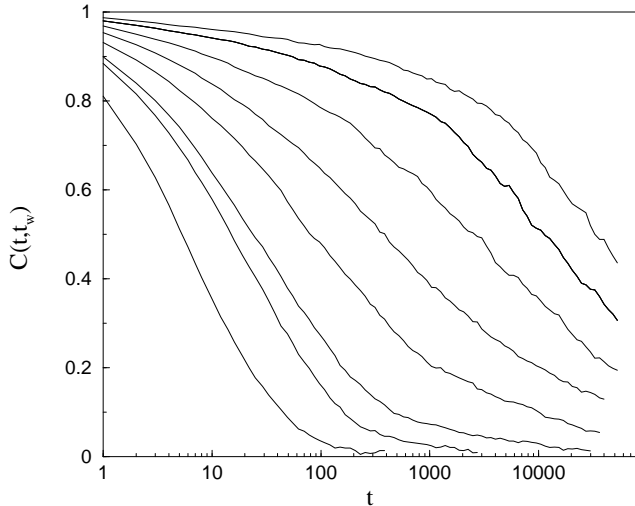


FIG. 4. The spin autocorrelation function $C(t, t_w)$ in the glassy phase at temperature $T = 3.2$. Eight different different waiting times are shown. From bottom to top $t_w = 10, 100, 200, 500, 1000, 2000, 5000, 10000$.

However, simply having a strong waiting-time dependence in a two-time correlation function does not imply glassy behaviour. Indeed, simple coarsening systems exhibit aging [13]. To distinguish this type of dynamics, type I aging [14], from glassy dynamics, type II aging, we have considered the overlap distribution function

$$Q(t_w + t, t_w + t) = \frac{1}{N} \sum_i S_i^{(1)}(t + t_w) S_i^{(2)}(t + t_w). \quad (5)$$

This is measured by first relaxing the system from a disordered state for a time t_w . Then two copies of the system are made, $\{S_i^{(1)}\}$ and $\{S_i^{(2)}\}$, and each is evolved for a further time t with independent thermal noise.

In Fig. 5 we show a plot of $Q(t_w + t, t_w + t)$ vs. $C(t, t_w)$ for three different waiting times. In each case $Q(t_w + t, t_w + t) \rightarrow 0$ as $C(t, t_w) \rightarrow 0$, indicating that the two copies of the system continue to move apart from each other irrespective of when the copies were made. This behaviour is indicative of type II, glassy aging [14]. Note that this behaviour is not an automatic consequence of the existence of infinitely many ground states. For example, we expect that for a triangular lattice anti-ferromagnet, $Q(t_w + t, t_w + t)$ would tend to a constant as $C(t, t_w)$ tends to zero, despite the non-zero ground-state entropy per spin. Finally, we have observed that $C(t, t_w)$ and $Q(t_w + t, t_w + t)$ are related by $C(2t, t_w) = Q(t_w + t, t_w + t)$ over a wide range of timescales. This relation is known to hold in equilibrium, where both functions are independent of t_w [14]. It has also been verified in the aging regime of some trap mod-

els as well as in the spin-glass version of the plaquette model [15].

These results provide evidence that the free-energy landscape of the ferromagnetic plaquette model is indeed complex and has many mutually inaccessible minima. This property is similar to what is seen in structural glasses and in mean field spin-glass models.

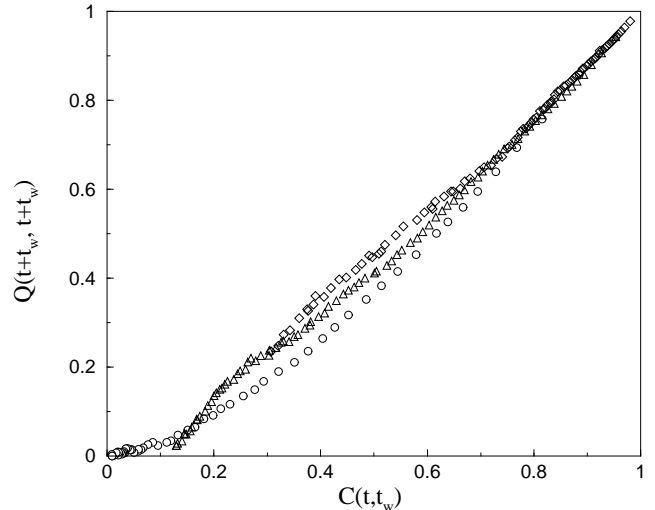


FIG. 5. Plot of $Q(t_w + t, t_w + t)$ versus $C(t, t_w)$. Three weighting times are shown: $t_w = 100(\circ), 1000(\triangle), 5000(\diamond)$.

VI. CONCLUSIONS

We have shown that the ferromagnetic plaquette model has many characteristics in common with glass forming liquids. We provided an explanation for the long-lived nature of the supercooled phase in terms of standard nucleation theory. By measuring the two-time correlation functions, we have observed two distinct kinds of behavior: (i) in the supercooled phase, the system appears to be stationary and the timescale of the energy autocorrelation functions diverges at a temperature identified in earlier work as a glass transition temperature T_g , and (ii) below T_g the spin-spin autocorrelation functions exhibit aging of a form characteristic of glasses. Our findings, along with the work reported in [4,5], indicate that a deeper understanding of this model would indeed be worthwhile.

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